1 Create a PSD file

This menu selection is used to create and store a particle size distribution (PSD) file which specifies the number of cement particles of each diameter to be placed in a starting 3-D microstructure. The output file created by this selection can be specified as input to the next submenu item, **Generate initial microstructure**.

Entering the **Create a PSD file** submenu takes the user to a form shown in Figure 1, which requires the user to select a cement from the local database. Choosing any cement from the cement database will load information about the PSD of that cement, i.e., the mass fraction as a function of particle diameter. For each cement, these data are stored in the cement images directory, in a subdirectory for that cement name, in a text file having a `.psd` extension.

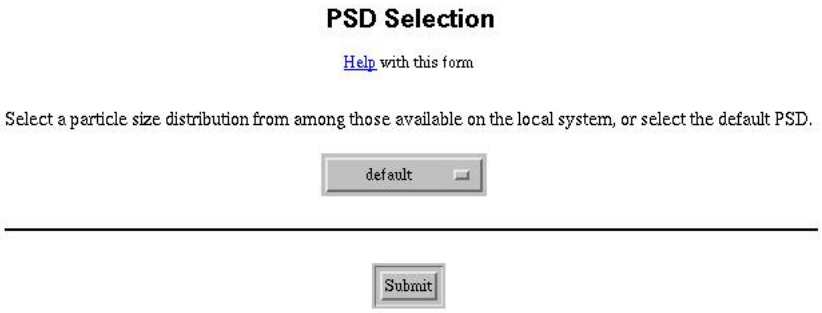

Figure 1: Form for selecting a cement PSD, system size, and system resolution.

Once the user submits this form, a second form is displayed. This form (shown in Figures 2 and 3) is used to actually specify PSD information, which will be written to a file. The components of the form are as follows:

1.1 Selected cement

To remind the user of the cement that was selected in the previous form, the name and an image of the cement is displayed at the top of the form, (see Figure 3), along with the chosen system size and resolution. A link is provided to return to the previous form if different settings are desired.

1.2 Particle specific gravity

The user may specify the specific gravity of the particles in question. This form may be used to create particle size distribution files for many different compounds that will be present in a cement powder. Entering the specific gravity here allows the connection between mass fraction and volume that is required to calculate the number of particles to include in each size class. Common values for the specific gravity for different components are provided in Table 1.

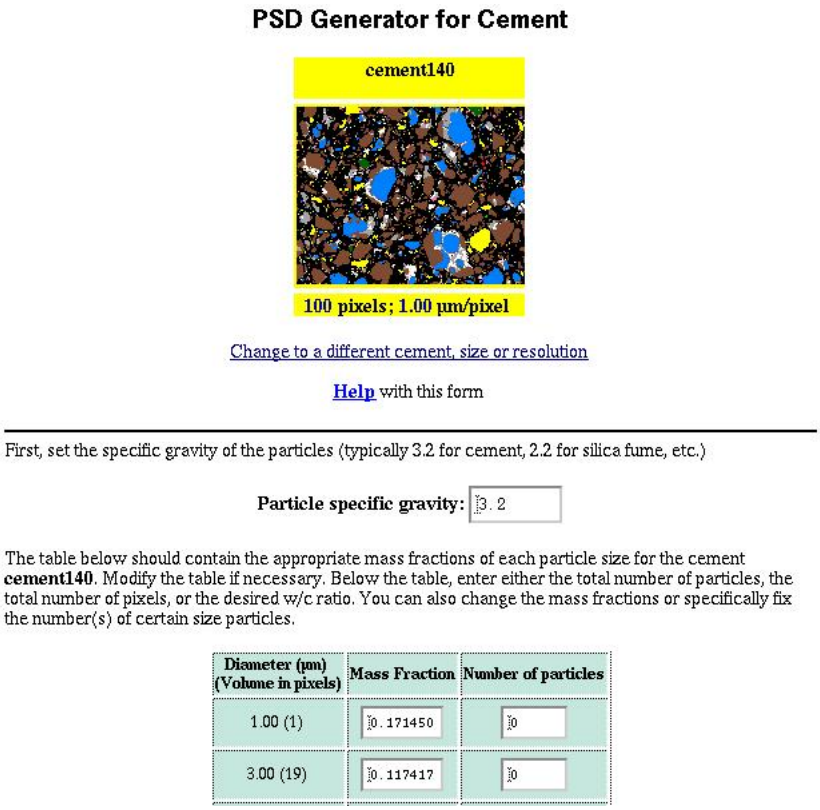

Figure 2: Top portion of the web form for creating a PSD file.

Compound/Phase	Specific Gravity	Compound/Phase	Specific Gravity
Cement clinker	3.2	Fumed silica	2.2
Corundum	3.97	Quartz	2.64
Fly Ash	2.55	Gypsum (dihydrate)	2.32
Hemihydrate (bassanite)	2.73	Anhydrite	2.61

Table 1: Specific gravity of common cement phases and admixtures.

1.3 PSD Table

This table lists the diameter, mass fraction, and number of particles for each size class. The mass fractions are taken directly from the cements database. The number of size classes (rows in the table) is determined by the values, entered on the previous form, for the system size and resolution. In particular, particle diameters (in pixels) that exceed 3/4 the system size are not allowed. Therefore, ordinarily they will not need to be edited, although they can be changed if the user desires. The user may enter the number of particles of each size class directly in this table, although this can be tedious and other methods are available (see below).

The final row of the PSD table contains the sums of each of the columns. The total mass fraction is present only to serve as a check that the sum of all the mass fractions is nearly unity; the value displayed in this field cannot be directly changed by the user, although a modification of one or more of the individual mass fractions will update its value.

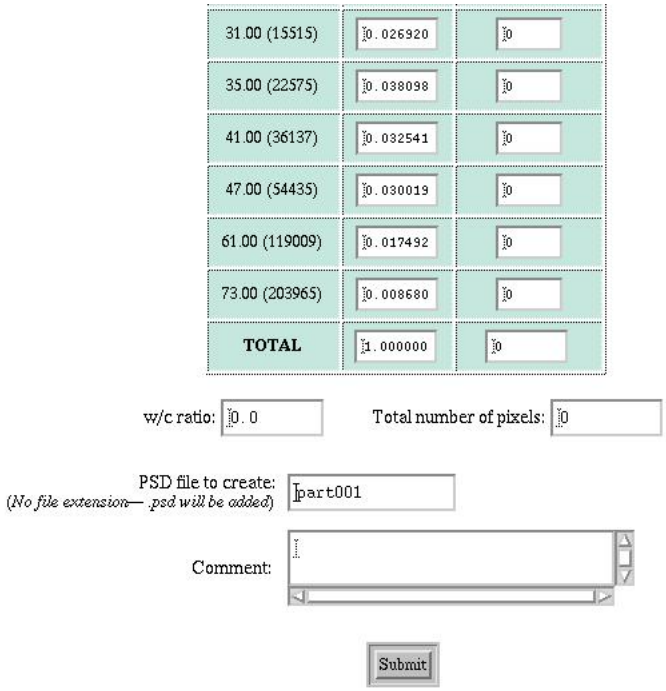

Figure 3: Bottom portion of the web form for creating a PSD file.

The other entry in the final row of the table is the total number of particles. This value **can** be directly specified by entering a positive integer in the appropriate text field. The numbers of particles of each size class will automatically adjust, according to the mass fractions, to meet the specified total. In most circumstances, however, the total number of particles has little importance compared to the water-cement ratio or the total number of solid pixels, either of which may be specified as described below. If the user *does* wish to specify the total, the value entered must not be so large that more than 80 % of the system pixels are solids.

1.4 w/c ratio

The user may request an approximate water-to-cement ratio here. Javascript code in the web page will automatically calculate the numbers of particles of each size class that most closely approximate that w/c. The number of particles and total number of pixels will also be updated. Note that the actual w/c ratio usually will not be equal to the value requested, because only whole numbers of particles of each size class are allowed. In particular, one too many large particles may result in a substantial decrease in the w/c. In this case, the user may manually set the mass fraction of these larger diameter particles to zero and repeat the automatic calculation by respecifying the desired value. Alternatively, if the intended simulations depend on the influence of coarse particles, or if the PSD of the cement is weighted heavily toward larger particles, then the user may manually decrease the numbers of smaller particles from several classes until the w/c ratio is closer to the desired value. This has limited impact if many large particles are required.

1.5 Total number of pixels

The user may request an approximate total number of solid pixels (not particles), and the embedded Javascript code will automatically calculate the numbers of particles of each size that most closely approximate that total. Note that the actual pixel total usually will not equal the value requested, because only whole numbers of particles of each size class are allowed.

Specifying the total number of pixels often comes in handy when the user is attempting to construct a blended cement from several different materials (e.g., flyash, pozzolans, inert fillers etc). If the PSD file for the clinker already has been created by specifying w/c ratio, and if the total number of cement pixels is therefore known, then PSD files for a subsequent component can be made by calculating the number of pixels of that component needed to achieve the desired volume fraction of solid and using that value to create the new PSD. A step-by-step example of this procedure for creating a blended cement microstructure is provided in Appendix A.

1.6 Name of the particle file

The data in the PSD table will be saved to a file for subsequent use in other calculations. Note that only the file root should be supplied (i.e., no file extension should be added) because the VCCTL software automatically appends the extension `.psd` to the name that is supplied. The file must have a unique name not already stored in the system; an error message will be displayed otherwise.

NOTE: It is highly recommended that a notebook be used to keep a record of the filenames used, as well as any other pertinent information that may help the user remember the context under which the files were created. The output from the web forms, which contains all such relevant information, can be printed and stored in such a notebook if desired.

1.7 User comment

The contents of this entry will be printed on the output page that is generated once the user submits this form. It exists to provide a reminder of the intent of the PSD file (e.g., what type of cement was selected, intended simulations, etc.)

1.8 Total mass fraction

This field keeps a running sum of the mass fractions. In almost all cases, its value should be unity, which ensures a normalized PSD. Values significantly less than unity might indicate an error in the program or that the user has changed the mass fractions in the table.

Once the form is complete and the "Submit" button is clicked, an output page is generated. The output page contains all the vital information that was used to create the PSD file, along with the file name and any comments that the user entered. It is recommended that this output page be printed out because it contains the only record of the file name and any comments that the user included. The current version of VCCTL does *not* provide reminders of the available PSD file names later on. If the output page is not printed out and the information needed later is forgotten,

write down as much information as possible, including the approximate date and time the file was created, and what it *might* be named. Then the directory ~`vcctl/data` can be searched manually using the `ls` command. For example, if the desired PSD file is thought to include "cem" in its name, execute the command

```
ls -alF ~vcctl/data/*cem*.psd
```

at the command prompt to display a list of all such files. From the list, one may identify the correct file from the date that it was created.

References